

Chemical Engineering Design II CHE-S401



Multicomponent Distillation

- Multicomponent distillations are more complicated than binary systems.
- Actual or potential involvement or interaction of one or more components of the multicomponent system on other components of the mixture.
- These interactions may be in the form of vapor-liquid equilibria such as azeotrope formation, or chemical reaction, etc.
- Any of these may affect the activity relations, and hence deviations from ideal relationships.
- The problem of determining the stage and reflux requirements for multicomponent distillations is also more complex than for binary mixtures.
- Multicomponent mixture, fixing one component composition does not uniquely determine the other component compositions and the stage temperature.

- The feed contains more than two components, it is not possible to specify the complete composition of the top and bottom products independently.
- The separation between the top and bottom products is specified by setting limits on two “key” components, (light and heavy key) between which it is desired to make the separation.

light key is the most volatile component whose concentration is to be controlled in the bottom product.

heavy key is the least volatile component whose concentration is to be controlled in the overhead product.

- The normal procedure to deal with this complexity of multicomponent distillation calculations are done by solving the MESH equations stage-by-stage, from the top and bottom of the column toward the feed point.

MESH: Material balance, Equilibrium, Summation, and Heat (energy) balance equations.

- The greater the number of components, the more difficult the problem.
- For other than ideal mixtures, the calculations will be further complicated by the fact that the component volatilities will be functions of the unknown stage compositions.
- If more than a few stages are required, stage-by-stage calculations are complex and tedious.
- Before the advent of the modern digital computer, various “shortcut” methods were developed to simplify the task of designing multicomponent columns.
- The shortcut methods available can be divided into two classes:
 1. Simplification of the rigorous stage-by-stage procedures to enable the calculations to be done by hand or graphically. Typical examples of this approach are the methods given by Smith and Brinkley (1960) and Hengstebeck (1976).

- Empirical methods, which are based on the performance of operating columns, or the results of rigorous designs. Typical examples of these methods are Gilliland's correlation, which is given in Richardson et al. (2002), and the Erbar-Maddox correlation.

Key Components

- The two components in a feed mixture whose separations will be specified.
 1. Adjacent keys: key components that are adjacent with respect to their volatilities.
 2. Split keys: key components that are separated in volatilities by a non-key component, i.e., the system of components contains one or more whose volatilities fall between the volatilities of the designated keys.
 3. Light key: the designation of the key component with the highest volatility of the two key components.
 4. Heavy key: the designation of the key component with the lowest volatility of the two key components.

- Example: component designations

Component	Relative Volatility $\alpha_{l/h}$ -7°F. and 550 psia	Designation
Hydrogen	11.7	Lighter than Key
Methane	3.7, α_l	Light <i>Keq</i> , l
Ethylene	1.0, α_h	<i>Heavy Keq</i> , h
Ethane	0.72	Heavier than Key
Propylene	0.23	Heavier than Key
Propane	0.19	Heavier than Key

If close boiling isomers are present, judgment must be used in their selection.

- The nonkey components that appear in both top and bottom products are known as **distributed components**;
- Those that are not present, to any significant extent, in one or another product, are known as **nondistributed components**.

- In multicomponent distillations it is not possible to obtain more than one pure component, one sharp separation, in a single column.
- If a multicomponent feed is to be split into two or more virtually pure products, several columns will be needed.
- Impure products can be taken off as side streams, and the removal of a side stream from a stage reduce the concentration of that component in the main product.
- The number of possible ways of separating components goes up sharply with the number of products.

For example:

From two arrangements with three products to more than 100 with seven products.

Five possible arrangements for separating four components with three columns.

Column 1		Column 2		Column 3	
Ovhd	Btms	Ovhd	Btms	Ovhd	Btms
A	BCD	B	CD	C	D
A	BCD	BC	D	B	C
AB	CD	A	B	C	D
ABC	D	A	BC	B	C
ABC	D	AB	C	A	B

Heuristic Rules for Optimum Sequencing

1. Remove the components one at a time; as in the benzene-toluene-xylene.
2. Remove any components that are present in large excess early in the sequence.
3. With difficult separations, involving close boiling components, postpone the most difficult separation to late in the sequence.

Difficult separations will require many stages, so the column diameter should be made as small as possible by adjusting flow rate to reduce cost.

Tall Columns

- When a large number of stages is required, then split a column into two separate columns to reduce the height of the column, even though the required separation could, theoretically, have been obtained in a single column.
- This may also be done in vacuum distillations, to reduce the column pressure drop and limit the bottom temperatures.

Number of Free Variables

- The performance of a given column or the equipment requirements for a given separation are established by solution of certain mathematical relations.

For a separation of C components in a column of n trays,

Item	Name	Number of Variables
1	feed rate	1
2	feed composition	$C - 1$
3	feed enthalpy	1
4	ratio of overhead and feed rates	1
5	reflux enthalpy	1
6	reflux ratio, L/D or L/V	1
7	number of trays	1
8	column pressure	1
		$C + 6$

Multicomponent Distillation

Shortcut Methods For Stage And Reflux Requirements

- Most of the **shortcut methods** were developed for the **design of separation columns for hydrocarbon systems** in the petroleum and petrochemical systems industries.
- When applying them to **other systems**. They usually depend on the **assumption of constant relative volatility** and should **not be used for severely nonideal systems**.
- Shortcut methods for nonideal and azeotropic systems are given by Featherstone (1971, 1973).

Pseudo-Binary Systems

- If the presence of the other components **does not** significantly affect the **volatility of the key components**, the keys can be treated as a **pseudo-binary pair**.
- The **number of stages** can then be calculated using a **McCabe-Thiele diagram** or the **other methods** developed for binary systems.
- This **simplification can often be made** when the **number of the nonkey components is small** or where the **components form near-ideal mixtures**.

- Where the **concentration of the nonkeys is small**, say less than 10%, they can be **lumped in with the key components**.
- For **higher concentrations** the method proposed by Hengstebeck (1946) can be used to **reduce the system to an equivalent binary system**.

Hengstebeck's Method

- For any component i , the Lewis-Sorel material balance equations and equilibrium relationship can be written in terms of the individual component molar flow rates, in place of the component composition:

$$v_{n+1,i} = l_{n,i} + d_i$$

$$v_{n,i} = K_{n,i} \frac{V}{L} l_{n,i}$$

- For stripping section $l'_{n+1,i} = v'_{n,i} + b_i$

$$v'_{n,i} = K_{n,i} \frac{V'}{L'} l'_{n,i}$$

where

$l_{n,i}$ = the liquid flow rate of any component i from stage n ;

$v_{n,i}$ = the vapor flow rate of any component i from stage n ;

d_i = the flow rate of component i in the tops;

b_i = the flow rate of component i in the bottoms;

$K_{n,i}$ = the equilibrium constant for component i at stage n .

The superscript ' denotes the stripping section.

V and L are the total flow rates, assumed constant.

- To reduce a multicomponent system to an equivalent binary, it is necessary to estimate the flow rate of the key components throughout the column.
- Hengstebeck makes use of the fact that in a typical distillation the flow rates of each of the light nonkey components approaches a constant, limiting rate in the rectifying section.
- The flows of each of the heavy nonkey components approach limiting flow rates in the stripping section.

Putting the flow rates of the nonkeys equal to these limiting rates in each section enables the combined flows of the key components to be estimated.

Rectifying section:

$$L_e = L - \sum \underline{l}_i$$

$$V_e = V - \sum \underline{v}_i$$

Stripping section: $L'_e = L' - \sum \underline{l}'_i$

$$V'_e = V' - \sum \underline{v}'_i$$

where

V'_e and L'_e are the estimated flow rates of the combined keys;

\underline{l}_i and \underline{v}_i are the limiting liquid and vapor rates of components lighter than the keys in the rectifying section;

\underline{l}'_i and \underline{v}'_i are the limiting liquid and vapor rates of components heavier than the keys in the stripping section.

The method used to estimate the limiting flow rates is that proposed by Jenny (1939).

The equations are

$$\underline{l}_i = \frac{d_i}{\alpha_i - 1}$$

$$\underline{v}_i = \underline{l}_i + d_i$$

$$\underline{v}'_i = \frac{\alpha_i b_i}{\alpha_{LK} - \alpha_i}$$

$$\underline{l}'_i = \underline{v}'_i + b_i$$

where

α_i = relative volatility of component i, relative to the heavy key (HK);

α_{LK} = relative volatility of the light key (LK), relative to the heavy key.

- Estimates of the flows of the combined keys enable operating lines to be drawn for the equivalent binary system.
- The equilibrium line is drawn by assuming a constant relative volatility for the light key:

$$y = \frac{\alpha_{LK}x}{1 + (\alpha_{LK} - 1)x}$$

where y and x refer to the vapor and liquid concentrations of the light key.

Smith-Brinkley Method

Method determine the distribution of components in multicomponent separation processes.

This method is based on the solution of the finite-difference equations that can be written for multistage separation processes and can be used for extraction and absorption processes, as well as distillation.

The derivation of the equations is given by Smith and Brinkley (1960) and Smith (1963).

For any component i (suffix i omitted in the equation for clarity)

$$\frac{b}{f} = \frac{(1 - S_r^{N_r - N_s}) + R(1 - S_r)}{(1 - S_r^{N_r - N_s}) + R(1 - S_r) + GS_r^{N_r - N_s}(1 - S_s^{N_s + 1})} \quad (1)$$

where

b/f is the fractional split of the component between the feed and the bottoms, and

N_r = number of equilibrium stages above the feed;

N_s = number of equilibrium stages below the feed;

S_r = stripping factor, rectifying section = $K_i V/L$;

S_s = stripping factor, stripping section = $K'_i V'/L'$;

V and L are the total molar vapor and liquid flow rates, and the superscript ' denotes the stripping section.

G depends on the condition of the feed.

If the feed is mainly liquid: $G_i = \frac{K'_i}{K_i} \frac{L}{L'} \left[\frac{1 - S_r}{1 - S_s} \right]_i$

and the feed stage is added to the stripping section.

- If the feed is mainly vapor:

$$G_i = \frac{L}{L'} \left[\frac{1 - S_r}{1 - S_s} \right]_i$$

Equ. (1) is for a column with a total condenser.

If a **partial condenser** is used, the **number of stages** in the rectifying section should be **increased by one**.

The procedure for using the Smith-Brinkley method is as follows:

1. Estimate the flow rates L , V and L' , V' from the specified component separations and reflux ratio.
2. Estimate the top and bottom temperatures by calculating the dew and bubble points for assumed top and bottom compositions.
3. Estimate the feed-point temperature.
4. Estimate the average component K values in the stripping and rectifying sections.
5. Calculate the values of $S_{r,i}$ for the rectifying section and $S_{s,i}$ for the stripping section.

6. Calculate the fractional split of each component and hence the top and bottom compositions.
7. Compare the calculated values with the assumed values and check the overall column material balance.
8. Repeat the calculation until a satisfactory material balance is obtained. The usual procedure is to adjust the feed temperature up and down until a satisfactory balance is obtained.

This method is basically a rating method, suitable for determining the performance of an existing column, rather than a design method, as the number of stages must be known.

It can be used for design if the number of stages estimated by some other method then use equ. (1) to determine the top and bottom compositions.

The estimated stages can then be adjusted and the calculations repeated until the required specifications are achieved.

The Geddes-Hengstebeck method for estimating the component splits is easier to use and satisfactory for preliminary design.

Empirical Correlations

- The two most frequently used empirical methods to estimate the stage requirements for multicomponent distillations are the correlations published by Gilliland (1940) and by Erbar and Maddox (1961).
- These methods relate the number of ideal stages required for a given separation, at a given reflux ratio, to the number at total reflux (minimum possible) and the minimum reflux ratio (infinite number of stages).
- Gilliland's correlation is given in Richardson et al. (2002).
- The Erbar-Maddox correlation is give more reliable predictions. Their correlation is shown in Figure, which gives the ratio of number of stages required to the number at total reflux, as a function of the reflux ratio, with the minimum reflux ratio as a parameter.
- To use this Figure, estimates of the number of stages at total reflux and the minimum reflux ratio are needed.

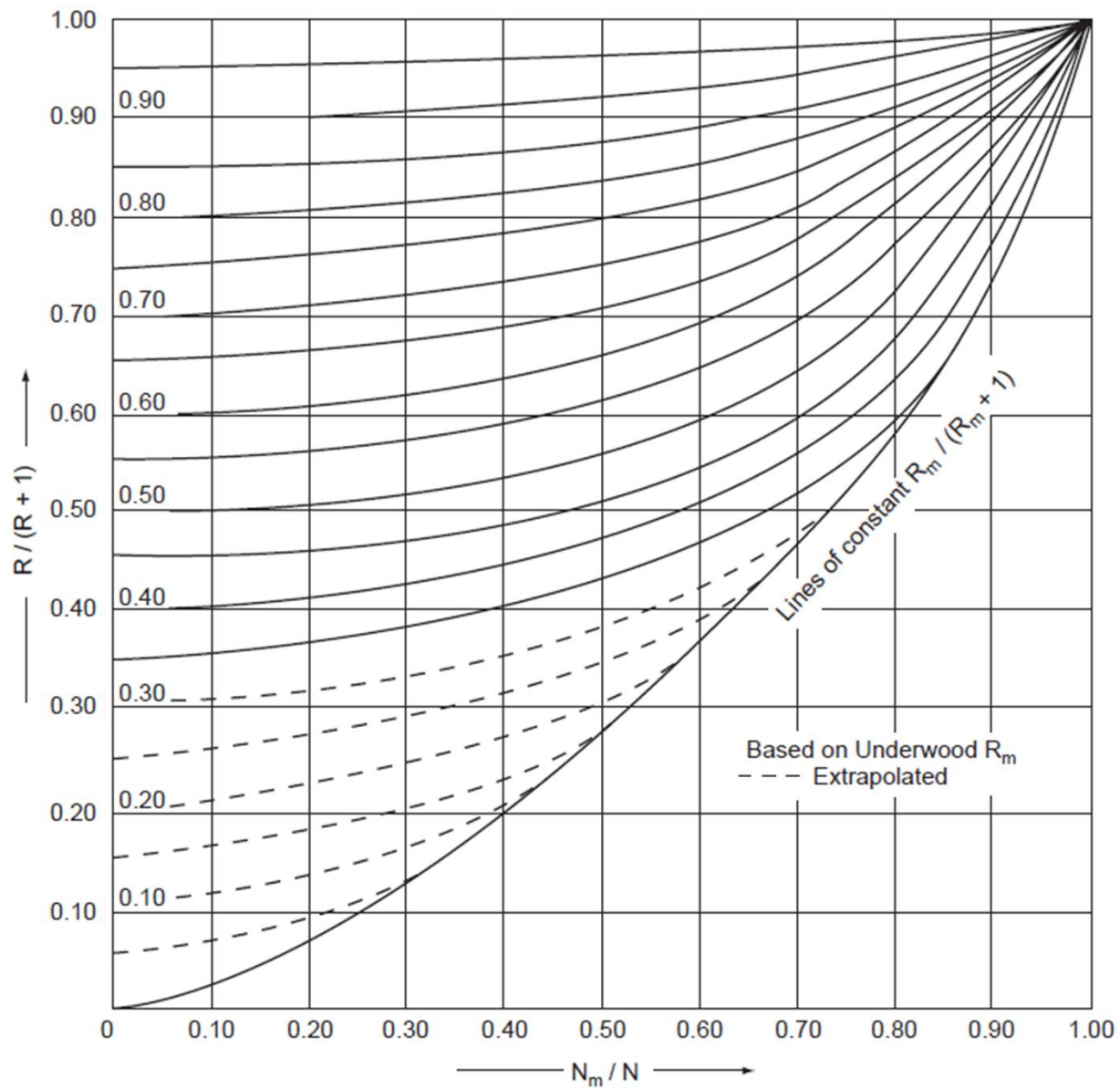


Figure Erbar-Maddox correlation (Erbar and Maddox, 1961).

Minimum Number of Stages (Fenske Equation)

- The Fenske equation (Fenske, 1932) can be used to estimate the minimum stages required at total reflux.
- The equation applies equally to multicomponent systems and can be written as

$$\left[\frac{x_i}{x_r} \right]_d = \alpha_i^{N_m} \left[\frac{x_i}{x_r} \right]_b$$

where

$[x_i/x_r]$ = the ratio of the concentration of any component i to the concentration of a reference component r , and the suffixes d and b denote the distillate (tops) (d) and the bottoms (b);

N_m = minimum number of stages at total reflux, including the reboiler;

α_i = average relative volatility of the component i with respect to the reference component.

- The separation required will be specified in terms of the key components, and equation can be rearranged to give an estimate of the number of stages:

$$N_m = \frac{\log \left[\frac{x_{LK}}{x_{HK}} \right]_d \left[\frac{x_{HK}}{x_{LK}} \right]_b}{\log \alpha_{LK}}$$

where α_{LK} is the average relative volatility of the light key with respect to the heavy key,
 x_{LK} and x_{HK} are the light and heavy key concentrations.

The **relative volatility** is taken as the **geometric mean** of the values at the **column top and bottom temperatures**.

- If there is a **wide difference between the relative volatilities** at the **top and bottom of the column**, the use of the **average value** in the Fenske equation will **underestimate the number of stages**.
- A **better estimate** can be made by **calculating the number of stages in the rectifying and stripping sections separately**.
- For **estimation of average relative volatilities** taking the **feed concentration as the base concentration** for the rectifying section and the **top concentration** for the stripping section.

This procedure will also give an estimate of the feed point location.

If the **number of stages is known**, equation can be **used to estimate the split of components between the top and bottom of the column at total reflux**. It can be written as:

$$\frac{d_i}{b_i} = \alpha_i^{N_m} \left[\frac{d_r}{b_r} \right]$$

where

d_i and b_i are the flow rates of the component i in the distillate and bottoms;

d_r and b_r are the flow rates of the reference component in the distillate and bottoms.

From the column material balance

$$d_i + b_i = f_i$$

where f_i is the flow rate of component i in the feed.

Minimum Reflux Ratio

Colburn (1941) and Underwood (1948) have given equations to estimate the minimum reflux ratio for multicomponent distillations.

Underwood equation is more widely used, The equation can be stated in the form

$$\sum \frac{\alpha_i x_{i,d}}{\alpha_i - \theta} = R_m + 1$$

where

α_i = the relative volatility of component i with respect to some reference component, usually the heavy key;

R_m = the minimum reflux ratio;

$x_{i,d}$ = concentration of component i in the tops at minimum reflux;

θ is the root of the equation:

$$\sum \frac{\alpha_i x_{i,f}}{\alpha_i - \theta} = 1 - q$$

where

$x_{i,f}$ = the concentration of component i in the feed, and q depends on the condition of the feed.

- The value of θ must lie between the values of the relative volatility of the light and heavy keys, and is found by trial and error.
- In these equations the relative volatilities are taken as constant. The geometric average of values estimated at the top and bottom temperatures should be used.

Feed-Point Location

- A limitation of the Erbar-Maddox and similar empirical methods is that they do not give the feed-point location.
- An estimate can be made by using the Fenske equation to calculate the number of stages in the rectifying and stripping sections separately, but this requires an estimate of the feed-point temperature.

An alternative approach is to use the empirical equation given by Kirkbride (1944):

$$\log \left[\frac{N_r}{N_s} \right] = 0.206 \log \left[\left(\frac{B}{D} \right) \left(\frac{x_{f,HK}}{x_{f,LK}} \right) \left(\frac{x_{b,LK}}{x_{d,HK}} \right)^2 \right]$$

where

N_r = number of stages above the feed, including any partial condenser;

N_s = number of stages below the feed, including the reboiler;

B = molar flow bottom product;

D = molar flow top product;

$x_{f,HK}$ = concentration of the heavy key in the feed;

$x_{f,LK}$ = concentration of the light key in the feed;

$x_{d,HK}$ = concentration of the heavy key in the top product;

$x_{b,LK}$ = concentration of the light key if in the bottom product.

Distribution of Nonkey Components (Graphical Method)

- The graphical procedure proposed by Hengstebeck (1946), which is based on the Fenske equation, is a convenient method for estimating the distribution of components between the top and bottom products.
- Hengstebeck and Geddes (1958) have shown that the Fenske equation can be written in the form

$$\log\left(\frac{d_i}{b_i}\right) = A + C \log \alpha_i$$

Specifying the split of the key components determines the constants A and C in the equation.

The distribution of the other components can be readily determined by plotting the distribution of the keys against their relative volatility on log-log paper and drawing a straight line through these two points.



This document was created with the Win2PDF "print to PDF" printer available at <http://www.win2pdf.com>

This version of Win2PDF 10 is for evaluation and non-commercial use only.

This page will not be added after purchasing Win2PDF.

<http://www.win2pdf.com/purchase/>